

# Projected BCS Wave Functions for Low Dimensional Frustrated Spin Systems

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Non-magnetic ground states are a fascinating possibility allowed by the physics of quantum antiferromagnets. These states – which lack the classical periodical long-range order – can be stabilized whenever reduced dimensionality, a small spin value, and/or the presence of competing interactions lead to strong enough zero-point quantum fluctuations.

One dimensional or quasi-one dimensional spin-half Heisenberg antiferromagnets often have non-magnetic ground states. Indeed for the 1D nearest-neighbors Heisenberg model

$$(1) \quad \hat{\mathcal{H}} = J_1 \sum_{n.n.} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j$$

the exact solution due to Bethe [1] predicts the absence of *true* long-range antiferromag-

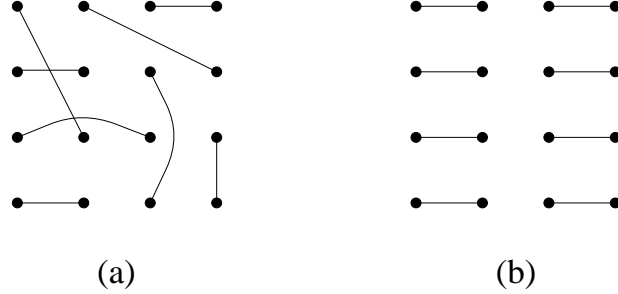


Fig. 1. – Sketch of a spin liquid (a) and of a symmetry-broken (b) non-magnetic RVB state. Each stick represents a singlet bond.

netic order even if the ground state is very close to have a broken symmetry, with a gapless excitation spectrum and a power-law decay of spin-spin correlations. This is also the case for any array consisting of an odd number of chains (odd-leg ladder systems). The ground state of two chains or in general of any even-leg ladder system is non-magnetic too. However – in contrast to the previous cases – here the correlation length is finite and the spectrum is gapped.[2] Such a gap is known to decrease exponentially with the number of legs [3] leading to a gapless spectrum in the two dimensional limit, where the ground state of the Heisenberg model has genuine long-range antiferromagnetic order.[4]

Competing interactions may allow in principle the stabilization of a non-magnetic ground state even in truly two dimensional systems. One of the simplest examples of these *frustrated* systems, which has been also recently realized experimentally [5], is the so-called  $J_1$ – $J_2$  model [6, 7]

$$(2) \quad \hat{\mathcal{H}} = J_1 \sum_{n.n.} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + J_2 \sum_{n.n.n.} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j ,$$

where the antiferromagnetic alignment between neighboring spins (due to  $J_1 > 0$ ) is hindered by a next-nearest-neighbors antiferromagnetic coupling ( $J_2 > 0$ ).

Classically, the minimum energy configuration of the 2D  $J_1$ – $J_2$  model has the conventional Néel order with magnetic wave vector  $\mathbf{Q} = (\pi, \pi)$  for  $J_2/J_1 < 0.5$ . Instead for  $J_2/J_1 > 0.5$  the minimum energy configuration is the so-called *collinear* state with the spins ferromagnetically aligned in one direction and antiferromagnetically in the other, corresponding to magnetic wave vectors  $\mathbf{Q} = (\pi, 0)$  or  $\mathbf{Q} = (0, \pi)$ . [8] Exactly at  $J_2/J_1 = 0.5$  any classical state having zero total spin on each elementary square plaquette is a minimum of the total energy. These states include both the Néel and the collinear states but also many others with no long-range order so that the occurrence of a non-magnetic ground state in the quantum case, for a small spin value, is likely around this value of the  $J_2/J_1$  ratio. Indeed, at present there is a general consensus on the fact that the combined effect of frustration and zero-point motion leads to the disappearance

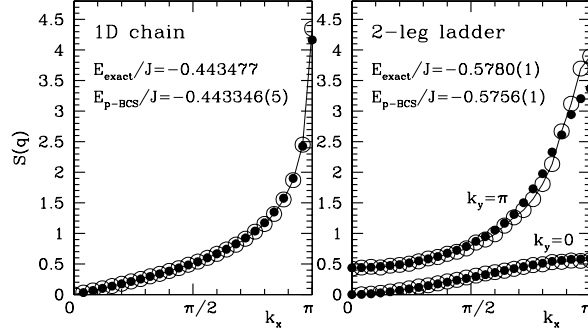


Fig. 2. – Variational estimate of the magnetic structure factor for the spin-half Heisenberg chain and two-leg ladder (filled circles). Empty dots are the numerically exact results obtained with the Green’s function Monte Carlo method.[22]

of the long-range antiferromagnetic order marked by the opening of a finite spin gap for  $\sim 0.4 < J_2/J_1 < \sim 0.55$ . [9, 10] The nature of this non-magnetic ground state is one of the most interesting puzzles of the physics of frustrated spin systems. In particular an open question is whether the ground state of the  $J_1$ – $J_2$  Heisenberg model is a homogeneous spin liquid, i.e., a state with all the symmetries of the Hamiltonian, as it was originally suggested by Figueirido *et al.* [11]. The other possibility is a ground state which is still  $SU(2)$  invariant, but nonetheless breaks some crystal symmetries, dimerizing in some special pattern (see below). [12, 13, 14, 15, 16, 10]

A simple picture of a non-magnetic ground state can be given in terms of the so-called *Resonating Valence Bond* (RVB) states.[17] These are linear superpositions of valence bond states in which each spin forms a singlet bond with another spin on the opposite sublattice (say  $A$  and  $B$ ) [18]

$$(3) \quad |\psi_{RVB}\rangle = \sum_{i_\alpha \in A, j_\beta \in B} h(r_1) \dots h(r_{N/2}) (i_1 j_1) \dots (i_{N/2} j_{N/2}) ,$$

where  $N$  is the number of sites of the lattice,  $r_m$  is the distance between the spins forming the  $m^{th}$  singlet bond  $(i_m j_m)$ , and  $h(r_m)$  is a bond weight factor. These states form in general a (overcomplete) basis of the  $S = 0$  subspace so that any singlet wave function can be represented in terms of them. However, they represent a non-magnetic state whenever the short-ranged bonds dominate the superposition (3). More precisely, it has been numerically shown by Liang, Doucot and Anderson[18] that the RVB state (3) has no long-range antiferromagnetic order for bonds that decay as rapidly as  $h(r) \sim r^{-p}$ , with  $p \geq 5$ . Such bonds can be either homogeneously spatially distributed on the lattice, with short-range correlations among each other (spin liquid) [fig. 1 (a)], or they can break some symmetries of the Hamiltonian, with the dimers frozen in some special patterns [fig. 1 (b)] as originally predicted for the  $J_1$ – $J_2$  model in the regime of strong frustration.

[12, 13, 14, 15, 16, 10]

In a seminal paper,[19] Anderson proposed that a physically transparent description of a RVB state can be obtained in fermionic representation by starting from a BCS-type pairing wave function, of the form

$$(4) \quad |\psi_{\text{BCS}}\rangle = \exp \left( \sum_{i,j} f_{i,j} \hat{c}_{i,\uparrow}^\dagger \hat{c}_{j,\downarrow}^\dagger \right) |0\rangle .$$

This wave function is the ground state of the well-known BCS Hamiltonian

$$(5) \quad H_{\text{BCS}} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_k (\Delta_k c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + h.c.)$$

where  $\sigma = \uparrow, \downarrow$ ,  $\epsilon_k = -2[\cos k_x + \cos k_y]$  is the free-electron dispersion and  $\Delta_k = \Delta_{-k}$  is the (real) gap function, provided the Fourier transform  $f_k$  of the pairing function,  $f_{i,j}$ , satisfies:  $f_k = \Delta_k / (\epsilon_k + \sqrt{\epsilon_k^2 + \Delta_k^2})$ . The non-trivial character of this wave function emerges when we restrict to the subspace of fixed number of electrons (equal to the number of sites) and enforce Gutzwiller projection onto the subspace with no double occupancies: singlet pairs do not overlap in real space and this wave function can be described by a superposition of valence bond states of the form (3).[19, 20, 21]

This *projected*-BCS (*p*-BCS) wave function turns out to be an almost exact representation of several low-dimensional spin system with non-magnetic ground states. For instance it provides an excellent variational ansatz of the ground state of the Heisenberg chain and of the two-leg ladder giving a very accurate estimate of the ground-state energy (fig. 2) and reproducing almost exactly the antiferromagnetic correlations. In the first case the spin structure factor  $S(q) = \langle \hat{\mathbf{S}}_q \cdot \hat{\mathbf{S}}_{-q} \rangle$  shows a cusp at  $q = \pi$  while for two-leg ladders it has a broad maximum at  $q = (\pi, \pi)$ . These features are remarkably well reproduced by the (*p*-BCS) variational wave function (fig. 2), which generates robust antiferromagnetic correlations at short distances with a very simple parameterization of the gap function:  $\Delta_k = \Delta_1 \cos k + \Delta_2 \cos 3k$  for the chain and  $\Delta_k = \Delta_x \cos k_x + \Delta_y \cos k_y$  for the ladder.[22]

In two dimensions this wave function has been already studied for the pure Heisenberg model by several authors[20, 21] for  $\Delta_k \propto (\cos k_x - \cos k_y)$ . In this case it provides a reasonable prediction for the ground-state energy but it fails in reproducing correctly the long-range antiferromagnetic order of the ground state. Here we show that this type of RVB state represents an extremely accurate variational ansatz for the  $J_1 - J_2$  model in the non-magnetic phase when the gap function  $\Delta_k$  is carefully parameterized. In particular, a definite symmetry is guaranteed to the *p*-BCS state provided  $\Delta_k$  transforms according to a one dimensional representation of the spatial symmetry group. A careful analysis [23, 24] shows that the odd component of the gap function  $\Delta_k = -\Delta_{k+(\pi,\pi)}$  may have spatial symmetries different from those of the even component  $\Delta_k = \Delta_{k+(\pi,\pi)}$ . Indeed, the best variational energy is obtained when the former has  $d_{x^2-y^2}$  symmetry, whereas the latter either vanishes or it has  $d_{xy}$  symmetry. In order to determine the best variational

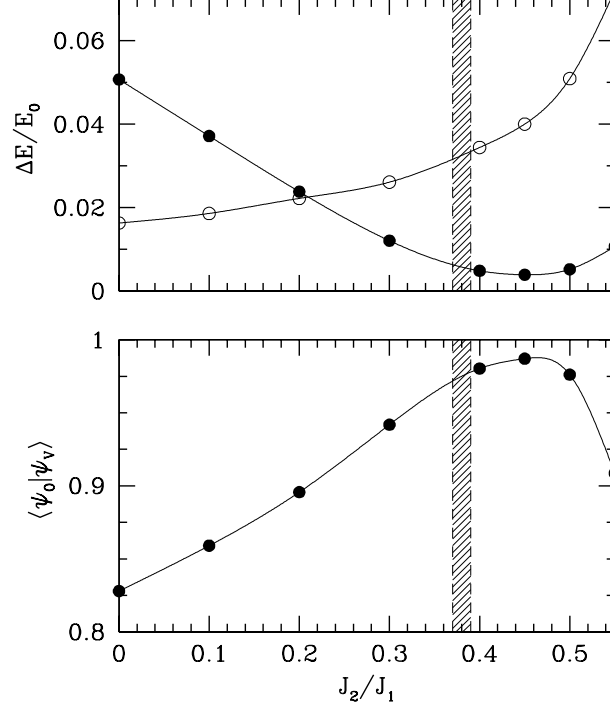


Fig. 3. – Accuracy of the ground-state energy, and overlap between the ground state and the  $p$ -BCS state (full dots) as a function of  $J_2/J_1$ , for  $N = 6 \times 6$ . Empty dots are the energy accuracy of a Néel ordered spin-wave wave function.[26, 7] Lines are guides for the eye and the shaded region indicates the location of the expected transition point to the non-magnetic phase.

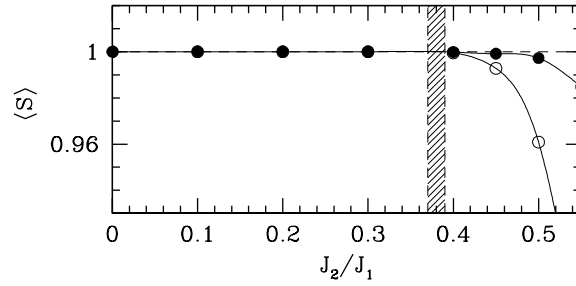


Fig. 4. – Average sign of the  $p$ -BCS state (full dots) as a function of  $J_2/J_1$ , for  $N = 6 \times 6$ . Empty dots are the Marshall sign obtained with the  $p$ -BCS state with only the  $d_{x^2-y^2}$  component of the gap function. Lines are guides for the eye and the shaded region indicates the location of the expected transition point to the non-magnetic phase.

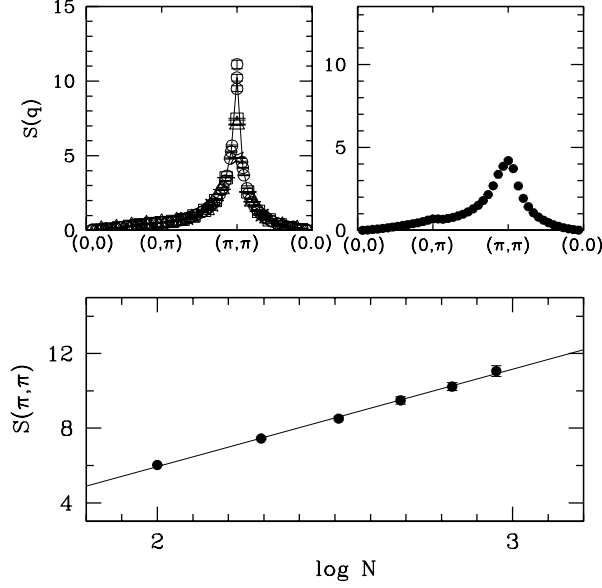


Fig. 5. – Antiferromagnetic structure factor of the  $d_{x^2-y^2}$  (top left panel) and  $d_{x^2-y^2} + d_{xy}$  (top right panel)  $p$ -BCS wave functions. Lower panel: size scaling of  $S(\pi, \pi)$  for the  $d_{x^2-y^2}$   $p$ -BCS state.

wave function of this form we have used a recently developed quantum Monte Carlo technique [25] that allows to optimize a large number of variational parameters with modest computational effort.

The remarkable accuracy of the  $p$ -BCS wave function in describing the ground state of the 2D  $J_1-J_2$  model in the regime of strong frustration can be shown by calculating the variational energy and the overlap with the exact ground state,  $|\psi_0\rangle$ , for the largest square cluster  $N = 6 \times 6$  where the solution can be numerically determined by exact diagonalization. As shown in fig. 3 the accuracy of the  $p$ -BCS wave function rapidly increase by increasing the frustration ratio  $J_2/J_1$  whereas conventional Néel ordered spin-wave wave functions [26, 7] quickly become less and less accurate. Entering the regime of strong frustration  $J_2/J_1 \sim 0.45 \pm 0.05$ , where a gapped non-magnetic ground state is expected, the  $p$ -BCS wave function becomes impressively accurate with a relative accuracy on the ground-state energy of order  $\sim 4 \times 10^{-3}$  and an overlap to the exact ground state of  $\sim 99\%$ , both improved by more than an order of magnitude with respect to the  $J_2 = 0$  case. This fact implies that the ground state in the strongly frustrated regime is almost exactly reproduced by a RVB wave function.

Interestingly, the transition to the regime of strong frustration is marked by the stabilization at the variational level of a non-zero  $d_{xy}$  component of the gap function. This allows to reproduce correctly the phases of the actual ground-state configurations as illustrated in fig. 4. A measure of the accuracy of a variational wave function  $|\psi_V\rangle$

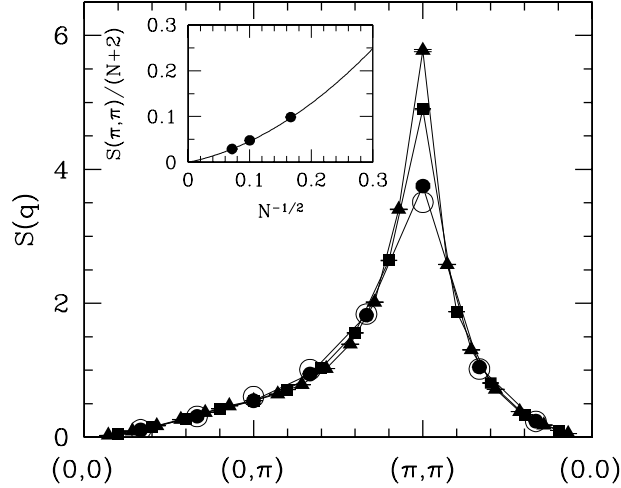


Fig. 6. – Variational estimate of  $S(q)$  for (from the lower to the upper curve)  $N = 6 \times 6$ ,  $10 \times 10$ , and  $14 \times 14$ . Large empty circles are the exact diagonalization results for the  $N = 6 \times 6$ . Inset: size-scaling of the order parameter squared.

in reproducing the phases of the ground state can be given in terms of the average sign  $\langle S \rangle = \sum_x |\langle x | \psi_V \rangle|^2 \text{Sgn}[\langle x | \psi_V \rangle \langle x | \psi_0 \rangle]$ . In the unfrustrated case it is well known that such phases are determined by the so-called Marshall sign rule [27]: on each real space configuration  $|x\rangle$ , the sign of the ground-state wave function is determined only by the number of spin down in one of the two sublattices. This feature, rigorously valid for  $J_2 = 0$ , turns out to be a very robust property for weak frustration ( $J_2/J_1 < \sim 0.3$ ). [28] However, it is clearly violated when frustration plays an important role. It can be shown [23, 24] that the Marshall sign (i.e.,  $\langle S \rangle = 1$  for  $J_2/J_1 = 0$ ) can be obtained using the  $p$ -BCS wave function, with only the  $d_{x^2-y^2}$  component, so that this wave function provides an almost exact representation of the ground-state phases for weak frustration. However, for  $J_2/J_1 > \sim 0.4$ , the phases of the wave function are considerably affected by the strong frustration and only when a sizable  $d_{xy}$  component is stabilized at the variational level, this property can be correctly reproduced.

An even more remarkable effect associated with the  $d_{xy}$  component of the gap function is the change induced on antiferromagnetic correlations. As it is shown, in fig. 5 the finite-size magnetic structure factor of the  $d_{x^2-y^2}$   $p$ -BCS state is sharply peaked around the antiferromagnetic wave vector  $\mathbf{Q} = (\pi, \pi)$  giving rise to a logarithmic divergence in the thermodynamic limit. Such a divergence is instead washed out in presence of the  $d_{xy}$  component of the gap function, leading to a state with weaker short-range antiferromagnetic correlations which is of course more suitable to describe the spin-gapped strongly-frustrated phase.

Of course, the accuracy in the energy does not necessarily guarantee a corresponding

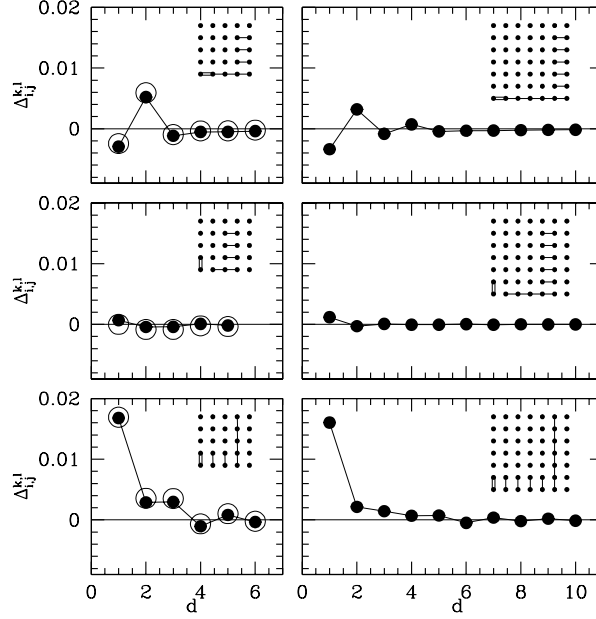


Fig. 7. – Variational estimate of the dimer-dimer correlation functions  $\Delta_{i,j}^{k,l}$  obtained by keeping fixed the position of the bond  $(i, j)$  (double stick) and moving the bond  $(k, l)$  (single stick) along the indicated patterns.  $d$  is the Manhattan distance.  $6 \times 6$  (left),  $10 \times 10$  (right). Large empty circles are the exact diagonalization results for the  $N = 6 \times 6$ .

accuracy in correlation functions. However, as shown in fig. 6, the comparison of the magnetic structure factor with the exact result gives a clear indication that correlation functions obtained by the variational approach are essentially exact. Furthermore using the stochastically implemented Lanczos technique and the variance extrapolation method [25] we have verified that the accuracy of the  $p$ -BCS wave function is preserved by increasing the lattice size.[23]

In order to investigate the existence of long-range dimer-like correlations, as in the columnar or the plaquette valence bond state, we have calculated the dimer-dimer correlation functions,  $\Delta_{i,j}^{k,l} = \langle \hat{S}_i^z \hat{S}_j^z \hat{S}_k^z \hat{S}_l^z \rangle - \langle \hat{S}_i^z \hat{S}_j^z \rangle \langle \hat{S}_k^z \hat{S}_l^z \rangle$ . In presence of some broken spatial symmetry, the latter should converge to a finite value for large distance. This is clearly ruled out by our results, shown in fig. 7, with a very robust confirmation of the *liquid* character of the ground state for  $J_2/J_1 \simeq 0.5$ , which is correctly described by our variational approach.

A totally symmetric spin-liquid solution proposed for this model in ref. [11] was actually rather unexpected after the work of Read and Sachdev,[14] providing arguments in favor of spontaneous dimerization. This conclusion was supported by series expansion [16, 10] and quantum Monte Carlo studies included the one done by two of us.[9] It is



clear however that it is very hard to reproduce a fully symmetric spin liquid ground state, with any technique, numerical or analytical, based on reference states explicitly breaking some lattice symmetry.

In conclusion, the spin-liquid RVB ground state, originally proposed to explain high-Temperature superconductivity, is indeed a very robust property of strongly frustrated low-dimensional spin systems. Due to the success in reproducing the non-magnetic ground states of other low-dimensional spin systems like the 1D chain and the two-leg ladder, [22] we expect that the  $p$ -BCS RVB wave function represents the *generic* variational state for a spin-half spin liquid, once the pairing function  $f_{i,j}$  is exhaustively parameterized according to the symmetries of the Hamiltonian. Work is in progress on this line of research.[24, 29]

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## REFERENCES

- [1] Bethe H., Z. Phys, **71** (1931) 205.
- [2] Dagotto E. and Rice T.M., Science, **271** (1996) 618.
- [3] Dell’Aringa S., Ercolessi E., Morandi G., Pieri P., and Roncaglia M., Phys. Rev. Lett., **78** (1997) 2457.
- [4] Reger J. D. and Young A.P., Phys. Rev. B, **37** (1988) 5978. Manousakis E., Rev. Mod. Phys., **63** (1991) 1; Sandvik A., Phys. Rev. B, **56** (1997) 11678; Calandra M. and Sorella S., Phys. Rev. B, **57** (1998) 11446.
- [5] Melzi R., Carretta P., Lascialfari A., Mambrini M., Troyer M., Millet P., and Mila F., Phys. Rev. Lett., **85** (2000) 1318; Carretta P., Melzi R., Papinutto N., and Millet P., Phys. Rev. Lett., **88** 47601 (2002); Carretta P., Papinutto N., Azzoni C.B., Mozzati M.C., Pavarini E., Gonthier S., Millet P., e.print cond-mat/0205092.
- [6] Chandra P. and Doucot B., Phys. Rev. B, **38** (1988) 9335.
- [7] for a review article see for instance Capriotti L., Int. J. Mod. Phys. B, **15** (2001) 1799.
- [8] Chandra P., Coleman P., and Larkin A.I., Phys. Rev. Lett., **64** (1990) 88.
- [9] Capriotti L. and Sorella S., Phys. Rev. Lett., **84** (2000) 3173.
- [10] Kotov V.N., Oitmaa J., Sushkov O., and Weihong Z., Phil. Mag. B, **80** (2000) 1483.
- [11] Figueirido F., Karlhede A., Kivelson S., Sondhi S., Rocek M., and Rokhsar D.S., Phys. Rev. B, **41** (1989) 4619.
- [12] Dagotto E. and Moreo A., Phys. Rev. Lett., **63** (1989) 2148.
- [13] Gelfand M. P., Singh R.R.P., and Huse D.A., Phys. Rev. B, **40** (1989) 10801.
- [14] Read N. and Sachdev S., Phys. Rev. Lett., **66** (1991) 1773.
- [15] Zithomirski M. and Ueda K., Phys. Rev. B, **54** (1996) 9007.
- [16] Singh R.R.P., Weihong Z., Hamer C.J., and Oitmaa J., Phys. Rev. B, **60** (1999) 7278.
- [17] Fazekas P. and Anderson P.W., Philos. Mag., **30** (1974) 423.
- [18] Liang S., Doucot B., and Anderson P.W., Phys. Rev. Lett., **61** (1988) 365.
- [19] Anderson P.W., Science, **235** (1987) 1196.
- [20] Gros C., Phys. Rev. B, **38** (1988) 931.

- [21] Poilblanc D., Phys. Rev. B, **39** (1989) 140.
- [22] Sorella S., Martins G.B., Becca F., Gazza C., Capriotti L., Parola A., and Dagotto E., Phys. Rev. Lett., **88** (2002) 117002.
- [23] Capriotti L., Becca F., Parola A., and Sorella S., Phys. Rev. Lett., **87** (2001) 097201.
- [24] Capriotti L. *et al.*, in preparation.
- [25] Sorella S., Phys. Rev. B, **64** (2001) 024512.
- [26] Franjic F. and Sorella S., Prog. Theor. Phys., **97** (1997) 399.
- [27] Marshall W., Proc. R. Soc. London Ser., **A 232** (1955) 48.
- [28] Richter J., Ivanov N.B., and Retzlaff K., Europhys. Lett., **25** (1994) 545.
- [29] Sorella S. *et al.*, in preparation.